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Electronic Properties of a Two-Dimensional Electron Gas at the Interface between Transition Metal Complex Oxides

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Abstract—The structural and electronic properties of heterostructures based on transition metal oxides containing strongly correlated electrons are compared. The investigated structures are $LaAlO_3/SrTiO_3$ (LAO/STO), $LaAlO_3/BaTiO_3$ (LAO/BTO), and $BaTiO_3/SrTiO_3$ (BTO/STO). The role of structural relaxation in the formation of a two-dimensional electron gas at the interface of two dielectrics is revealed. The contribution from different orbitals and atoms to conductivity is analyzed, along with the correlation between structural distortions induced by the dipole moment in an LAO layer and conductivity.

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In 2004, Ohtomo and Hwang [1] reported an observation of a high-mobility electron gas at an interface between $LaAlO_3$ (LAO) and $SrTiO_3$ (STO). Since then, heterointerfaces of these two nonconducting and nonmagnetic oxides have been observed in numerous studies. It was found that a metallic phase of nanometer thickness (a two-dimensional electron gas, 2DEG) forms in STO layers in structures with more than three LAO layers and interface LaO and TiO_2 layers. This phase becomes superconducting at temperatures below 300 mK [3]. The electron density in such heterostructures can be as high as 3×10^{13} cm^{-2}. In addition, ferromagnetism was observed in a LAO/STO heterostructure in [4].

Since STO is often used as a substrate, combinations of it and other compounds were examined in searching for emerging conductivity. A 2DEG was also observed at interfaces between other nonmagnetic dielectrics (e.g., $KTaO_3/SrTiO_3$ [5]). In addition, a 2DEG was found at the interface with antiferromagnetic $LaTiO_3$ [6] having a maximum density of 3×10^{14} cm^{-2}.

Several authors have assumed that the emergence of conductivity is related to structural (and thus electronic reconstructions), but a clear explanation and model of this phenomenon have yet to be presented. The aim of this work was therefore to examine the relationship between electronic correlations, structural distortions, and electronic reconstructions in LAO/STO and $LaAlO_3/BaTiO_3$ (LAO/BTO) heterostructures, which contain polar LaO and AlO_2 layers, and the BTO/STO heterostructure, in which the layers are electrically neutral but the emergence of ferroelectric polarization in BTO, which can switched as a result of external influences, may be expected.

The density functional theory approach [7] employed in VASP [8] was used as a research tool. Since strong correlations between the electrons of *d*-orbitals must be considered in modeling the electronic properties of transition metal oxides, we chose the GGA + *U* approximation for this, with corrections introduced as proposed by Dudarev [9]. Parameter *U*–*J* was added to the La 4*f* and Ti 3*d* orbitals ($U = 8$ and 2 eV, respectively). The magnetic nature of the material was ignored. Exchange and correlation effects were accounted for by using the GGA-PBE generalized gradient approximation [10]. Kohn–Sham equations were solved using the basis of plane waves (PAW) implemented in VASP, which was integrated into MedeA [11]. The cut-off energy was set at 400 eV, the residual forces were 0.05 eV Å^{-1}, and the energy convergence was 10^{-5} eV. The Brillouin zone was sampled using a $5 \times 5 \times 1$ grid.

The unit cell of heterostructures contained a central region of $SrTiO_3$ or $BaTiO_3$ (4.5 unit cells with boundary TiO_2 layers) surrounded from both sides by four $LaAlO_3$ layers with boundary LaO at the interface and AlO_2 at the surface (halves of unit cells are shown in Fig. 1). This structure ensured lack of polarity and a dipole moment induced by asymmetry. To avoid interaction between surfaces and their periodic copies, a 20 Å vacuum region was introduced into the calculations. Lattice constant $a = b = 3.905$ Å was taken from the experimental data for cubic bulk $SrTiO_3$. The experimental conditions of heterostructure growth were thus reproduced [1]. These lattice parameters